

NOV 27 2006

**Amendments to the Claims:**

This listing of claims will replace all prior versions and listings of claims in this application.

**Listing of Claims:**

1. (Cancelled).
2. (Cancelled).
3. (Currently Amended) A process for producing polyethylene using a slurry loop reactor comprising:

using a mathematical model to predict a plurality of process control parameters based on desired product properties and reactor characteristics and controlling the process using the predicted process control parameters;

wherein variables used to prepare the mathematical model include a plurality of variables selected from the group consisting of: ethylene flow into reactor, ethylene flow out of reactor, isobutane flow into reactor, isobutane flow out of reactor, hexene flow into reactor, hexene flow out of reactor, hexene conversion in reactor, hydrogen flow into reactor, hydrogen flow out of reactor, hydrogen conversion in reactor, polymer flow out of reactor, liquid flow out of reactor, total mass flow into reactor, total mass flow out of reactor, total volume flow out of reactor, catalyst flow into reactor, catalyst flow out of reactor, concentration of ethylene in the reactor liquid, concentration of hexene in the reactor liquid, concentration of hydrogen in the reactor liquid, temperature of reactor, pressure of reactor, weight concentration of solids in the reactor slurry, volume concentration of solids in the reactor slurry, weight concentration of solids in the settling leg solids bed, number of settling legs, reactor volume, settling leg diameter, settling leg height, bulk density of reactor polymer, density of reactor polymer, density of reactor liquid, density of reactor slurry, residence time of reactor solids, catalyst activity, catalyst productivity, catalyst diameter,

catalyst feed factor, catalyst activity factor, terminal velocity of settling polymer, polymer settling rate, rate of polymer leaving reactor that is not part of the settling leg solids bed, rate of slurry leaving reactor that is part of the settling leg solids bed, rate of slurry leaving reactor that is not part of the settling leg solids bed, viscosity of reactor liquid, density of catalyst, polymer diameter, Archimedes number for polymer settling in settling leg, Reynolds number for polymer settling in settling leg, acceleration due to gravity, cross sectional area of a settling leg occupied by polymer, and cross sectional area of a settling leg; and

wherein the variables used to prepare the mathematical model are: polymer flow out of the reactor, liquid flow out of the reactor, concentration of ethylene in the reactor liquid, temperature of the reactor, pressure of the reactor, weight concentration of solids in the reactor slurry, reactor volume, settling leg diameter, settling leg height, bulk density of the reactor polymer, density of the reactor polymer, and density of the catalyst.

4. (Currently Amended) A process for producing polyethylene using a slurry loop reactor comprising:

using a mathematical model to predict a plurality of process control parameters based on desired product properties and reactor characteristics and controlling the process using the predicted process control parameters;

wherein variables used to prepare the mathematical model include a plurality of variables selected from the group consisting of: ethylene flow into reactor, ethylene flow out of reactor, isobutane flow into reactor, isobutane flow out of reactor, hexene flow into reactor, hexene flow out of reactor, hexene conversion in reactor, hydrogen flow into reactor, hydrogen flow out of reactor, hydrogen conversion in reactor, polymer flow out of reactor, liquid flow out of reactor, total mass flow into reactor, total mass flow out of reactor, total volume flow out of reactor, catalyst flow into reactor, catalyst flow out of reactor, concentration of ethylene in the reactor liquid, concentration of hexene in the reactor liquid, concentration of hydrogen in the reactor liquid, temperature of reactor, pressure of reactor, weight concentration of solids in the reactor slurry, volume concentration of solids in the reactor slurry, weight concentration of solids in the settling leg solids bed, number of settling legs, reactor volume, settling leg diameter, settling leg height, bulk density of reactor polymer, density of reactor polymer, density of reactor liquid, density of reactor slurry, residence time of reactor solids, catalyst activity, catalyst productivity, catalyst diameter, catalyst feed factor, catalyst activity factor, terminal velocity of settling polymer, polymer settling rate, rate of polymer leaving reactor that is not part of the settling leg solids bed, rate of slurry leaving reactor that is part of the settling leg solids bed, rate of slurry leaving reactor that is not part of the settling leg solids bed, viscosity of reactor liquid, density of catalyst, polymer diameter, Archimedes number for polymer settling in settling leg, Reynolds number for polymer settling in settling leg, acceleration due to gravity, cross sectional area of a settling leg occupied by polymer, and cross sectional area of a settling leg; and

\_\_\_\_\_ wherein the variables used to prepare the mathematical model are: polymer flow out of the reactor, liquid flow out of the reactor, concentration of

ethylene in the reactor liquid, temperature of the reactor, pressure of the reactor, weight concentration of solids in the reactor slurry, reactor volume, settling leg diameter, settling leg height, bulk density of the reactor polymer, density of the reactor polymer, density of the catalyst, concentration of hexene in the reactor liquid, concentration of hydrogen in the reactor liquid, hexene conversion in the reactor, and hydrogen conversion in the reactor.

5. (Currently Amended) A process for producing polyethylene using a slurry loop reactor comprising:

using a mathematical model to predict a plurality of process control parameters based on desired product properties and reactor characteristics; and controlling the process using the predicted process control parameters; and

wherein the process is controlled using ~~the mathematical model variables selected from the group consisting of: mass balance of the reactor contents, reactor geometry, catalyst kinetics, and settling phenomena in the outlet settling legs, which is used to determine relationships between inlet feed rates and reactor geometry on production conditions, which has been incorporated into a computer spreadsheet.~~

6. (Cancelled).

7. (Currently Amended) A process for producing polyethylene using a slurry loop reactor comprising:

using a mathematical model to predict a plurality of process control parameters based on desired product properties and reactor characteristics and controlling the process using the predicted process control parameters;

wherein the process is controlled using the mathematical model comprised of variables selected from the group consisting of: mass balance of reactor contents, reactor geometry, catalyst kinetics, and settling phenomena in the outlet settling legs, which is used to determine relationships between inlet feed rates and reactor geometry on production conditions, and wherein said model which has been incorporated into a controller; and

wherein the controller is a neural network model based controller.

8.-11. (Cancelled).

12. (Currently Amended) A process for designing a configuration of a slurry loop reactor used to produce polymers comprising:

using a mathematical model to predict a plurality of process control parameters based on desired product properties and reactor characteristics and controlling the process using the predicted process control parameters, where variables used to prepare the mathematical model are selected from the group consisting of: mass balance of the reactor contents, reactor geometry, catalyst kinetics, and settling phenomena in the outlet settling legs, which is used to determine relationships between inlet feed rates and reactor geometry on production conditions; and

wherein have a variability is decreased by 70% in comparison to a conventional PID controller.

13. (New) The process of Claim 3, wherein the model is displayed in a spreadsheet.

14. (New) The process of Claim 4, wherein the model is displayed in a spreadsheet.
15. (New) The process of Claim 3, further comprising the steps of:
  - using sensors in the reactor to provide inputs to a PID controller;
  - using another controller to receive data from said PID controller; and
  - reprogramming the PID controller with the other controller, based upon the inputs from the reactor sensors.
16. (New) The process of Claim 15, wherein a plurality of PID controllers are used to receive inputs from the reactor sensors, and wherein the PID controllers are reprogrammed based upon the inputs from the reactor sensors and the other PID controllers.
17. (New) The process of Claim 3, wherein said mathematical model is incorporated into logic circuits of a controller.
18. (New) The process of Claim 4, wherein said mathematical model is incorporated into logic circuits of a controller.
19. (New) The process of Claim 3, wherein said mathematical model is created with a Fortran or C++ computer program.
20. (New) The process of Claim 4, wherein said mathematical model is created with a Fortran or C++ computer program.
21. (New) The process of Claim 7, wherein the model is displayed in a spreadsheet.

22. (New) A process for producing polyethylene using a loop reactor comprising:

using a mathematical model to predict a plurality of process control parameters based on desired product properties and reactor characteristics and controlling the process using predicted and actual process control parameters;

wherein the mathematical model includes settling leg data and a plurality of variables selected from the group consisting of:

$E_i$	=	ethylene flow into the reactor,
$E_o$	=	ethylene flow out of the reactor,
$I_i$	=	isobutane flow into the reactor,
$I_o$	=	isobutane flow out of the reactor,
$H_i$	=	hexene flow into the reactor,
$H_o$	=	hexene flow out of the reactor,
$H_c$	=	hexene conversion in the reactor,
$h_i$	=	hydrogen flow into the reactor,
$h_o$	=	hydrogen flow out of the reactor,
$h_c$	=	hydrogen conversion in the reactor,
$P_o$	=	polymer flow out of the reactor,
$L_o$	=	liquid flow out of the reactor,
$T_{iw}$	=	total mass flow into the reactor,
$T_{ow}$	=	total mass flow out of the reactor,
$T_{ov}$	=	total volume flow out of the reactor,
$C_i$	=	catalyst flow into the reactor,
$C_o$	=	catalyst flow out of the reactor,
$C_E$	=	concentration of ethylene in a reactor liquid,
$C_H$	=	concentration of hexene in a reactor liquid,
$C_h$	=	concentration of hydrogen in a reactor liquid,
$T$	=	temperature of the reactor,
$P$	=	pressure of the reactor,
$S_w$	=	weight concentration of solids in a reactor slurry,
$S_v$	=	volume concentration of solids in a reactor slurry,
$S_{ws}$	=	weight concentration of solids in a settling leg solids bed,
$N_i$	=	number of settling legs,
$V$	=	reactor volume,
$d_i$	=	settling leg diameter,
$h_i$	=	settling leg height,
$\rho_b$	=	bulk density of a reactor polymer,
$\rho_p$	=	density of a reactor polymer,
$\rho_l$	=	density of a reactor liquid,
$\rho_s$	=	density of a reactor slurry,
$t_s$	=	residence time of reactor solids,
$k$	=	catalyst activity,

$p$	=	catalyst productivity,
$d_c$	=	catalyst diameter,
$f_c$	=	catalyst feed factor,
$k_G$	=	catalyst activity factor,
$v_t$	=	terminal velocity of a settling polymer,
$P_s$	=	polymer settling rate,
$P_n$	=	rate of a polymer leaving the reactor that is not part of the settling leg solids bed,
$T_s$	=	rate of the slurry leaving the reactor that is part of the settling leg solids bed,
$T_n$	=	rate of the slurry leaving the reactor that is not part of the settling leg solids bed,
$m_l$	=	viscosity of the reactor liquid,
$r_c$	=	density of the catalyst,
$d_p$	=	polymer diameter,
$N_{Ar}$	=	Archimedes number for polymer settling in a settling leg,
$N_{Re}$	=	Reynolds number for polymer settling in a settling leg,
$g$	=	acceleration due to gravity,
$A_{lp}$	=	cross sectional area of a settling leg occupied by the polymer; and
$A_l$	=	cross sectional area of a settling leg.

23. (New) The process of Claim 22, wherein the mathematical model includes formulas selected from the group consisting of:

mass balance of a reactor, determined by:

$$T_{iw} - (L_o + P_o) = 0, \text{ where:}$$

$P_o$  is polymer flow out of the reactor,  $L_o$  is liquid flow out of the reactor, and  $T_{iw}$  is total mass flow into the reactor;

mass flows in an outlet liquid based upon outlet concentrations and hydrogen flow, determined by:

$$E_o = \frac{L_o C_E}{100}, H_o = \frac{L_o C_H}{100}, h_o = \frac{L_o C_h}{100}, I_o + E_o + H_o = L_o, \text{ and}$$

$$I_o = L_o - E_o - H_o, \text{ where:}$$

$E_o$  is ethylene flow out of the reactor,

$L_o$  is liquid flow out of the reactor,

$C_E$  is concentration of ethylene in the reactor liquid,

$H_o$  is hexene flow out of the reactor,

$C_H$  is concentration of hexene in the reactor liquid,



$C_h$  is concentration of hydrogen in the reactor liquid,  
 $h_o$  is hydrogen flow out of the reactor,  
 $I_o$  is isobutane flow out of the reactor, and  
 where  $h_o$  that is a smallest portion of total liquid flow;

an assumed mass balance of isobutane around the reactor, determined by:

$$I_i - I_o = 0, \text{ where:}$$

$I_i$  is isobutane flow into the reactor, and

$I_o$  is isobutane flow out of the reactor;

hexene and hydrogen feeds into the reactor, determined by:

$$H_o = \frac{H_i(100 - C_H)}{100}, H_i = \frac{100H_o}{100 - C_H}, h_o = \frac{h_i(100 - C_h)}{100}, \text{ and}$$

$$h_o = \frac{h_i(100 - C_h)}{100}, \text{ where:}$$

$H_i$  is hexene flow into the reactor,

$H_o$  is hexene flow out of the reactor, and

$C_H$  is concentration of hexene in the reactor liquid, wherein

a constant conversion of hexene and hydrogen into polymer across an intended operating region is assumed;

catalyst flow into the reactor, calculated using catalyst productivity and catalyst mass balance around the reactor, by:

$$p = \frac{P_o}{c_o} \text{ and } c_i - c_o = 0, \text{ where:}$$

$p$  is catalyst productivity,

$P_o$  is polymer flow out of the reactor,

$c_i$  is catalyst flow into the reactor, and

$c_o$  is catalyst flow out of the reactor;

slurry density, calculated using liquid density, an assumed polymer density, and a solids concentration, determined by:

$$\rho_s = \frac{100\rho_p\rho_l}{100\rho_p + S_w(\rho_l - \rho_p)};$$

volumetric flow rate of slurry out of the reactor determined from mass flow rate and density of each component, determined by:

$$T_{ov} = \frac{P_o}{\rho_p} + \frac{L_o}{\rho_l}$$

volumetric solids concentration in the reactor, determined by:

$$S_v = \frac{100}{1 + \frac{\rho_p}{\rho_l} \left( \frac{100}{S_w} - 1 \right)};$$

solid residence time, determined by:

$$\tau_s = \frac{V \rho_s S_w}{100 P_o};$$

catalyst activity, determined by:

$$p = \frac{P_o}{c_o} \text{ and } k = \frac{p}{\tau_s C_E};$$

a catalyst feed factor, determined by:

$$f_c = kc_i;$$

a catalyst feed factor, using a mass balance of catalyst around the reactor, determined by:

$$f_c = kc_i = kc_o = \frac{P_o}{\tau_s C_E};$$

a catalyst activity factor that quantifies reactivity of a catalyst with respect to the catalyst size, by:

$$k_c = \frac{k}{d_c^3};$$

concentration of a polymer in a settling bed as a function of the polymer, liquid densities, and polymer bulk density, determined by:

$$S_{wy} = \frac{100}{1 + \rho_l \left( \frac{1}{\rho_h} - \frac{1}{\rho_p} \right)};$$

mass balance of two portions of an outlet slurry, determined by:

$$T_{ow} = T_s + T_n;$$

mass balance of two portions of a polymer in outlet slurry, determined by:

$$P_o = P_s + P_n;$$

an amount of polymer leaving a settling leg from the settled bed of polymer, calculated using known polymer concentrations of two polymer portions, by:

$$T_s = \frac{100P_s}{S_{ws}}, T_n = \frac{100P_n}{S_w}, T_{ow} = \frac{100P_s}{S_{ws}} + \frac{100P_n}{S_w},$$

$$T_{ow} = \frac{100P_s}{S_{ws}} + \frac{100(P_o - P_s)}{S_w}, \text{ and } P_s = \frac{\frac{T_{ow}}{100} - \frac{P_o}{S_w}}{\frac{1}{S_{ws}} - \frac{1}{S_w}}, \text{ where:}$$

$T_s$  is the rate of slurry leaving the reactor that is part of the settling leg solids bed,  $T_n$  is the rate of slurry leaving reactor that is not part of the settling leg solids bed,  $T_{ow}$  is the total mass flow out of reactor, and wherein the flow rate indicates polymer settling rate in the settling leg;

viscosity of isobutane liquid as a function of temperature, determined by:

$$\mu_l(\text{cP}) = e^{-7.3891 + \frac{2582.6}{172.23 + T(\text{K})}};$$

polymer diameter, determined by:

$$d_p = 0.42d_c \left( \frac{\rho_c P}{\rho_p} \right)^{1/3};$$

Archimedes number for polymer settling through the isobutane liquid, determined by:

$$N_{Ar} = \frac{d^3 \rho_l g (\rho_p - \rho_l)}{\mu_l^2} \text{ and } N_{Ar} = 1.13e05;$$

calculation of a Reynolds number from the Archimedes number, by:

$$N_{Re} = \left( \sqrt{14.42 + 1.827 \sqrt{N_{Ar}}} - 3.798 \right)^2, \text{ then}$$

determining a velocity of a settling polymer, using:

$$N_{Re} = \frac{d_p v_i \rho_l}{\mu_l} \text{ and } v_i = \frac{N_{Re} \mu_l}{d_p \rho_l};$$

a mass flow of settling solids as related to a velocity of said solids, determined by:

$$P_s = N_l A_p v_i \rho_p;$$

an area of a settling leg occupied by polymer, determined by:

$$A_p = \frac{A_i S_v}{100} = \frac{\pi}{400} d_i^2 S_v.$$

then substituting said area of the settling leg into the mass flow of settling solids, determined by:

$$P_s = \frac{\pi}{400} N_l d_i^2 S_v v_i \rho_p; \text{ and}$$

wherein a number of settling legs required for reactor geometry and production conditions, is determined by:

$$N_l = \frac{400 P_s}{\pi d_i^2 S_v v_i \rho_p}.$$

24. (New) The process of Claim 22, wherein it is assumed that HDPE is produced from monomers consisting of ethylene and hexane, and where ethylene feed into the reactor is calculated from a mass balance of ethylene around the reactor, using:

$$E_i - \{E_o + [P_o - (H_i - H_o)]\} = 0 \text{ or } E_i = E_o + [P_o - (H_i - H_o)], \text{ where:}$$

$E_i$  is ethylene flow into the reactor,

$E_o$  is ethylene flow out of the reactor,

$P_o$  is polymer flow out of the reactor,

$H_i$  is hexene flow into the reactor, and

$H_o$  is hexene flow out of the reactor.

25. (New) The process of Claim 22, wherein it is assumed that HDPE is produced from monomers and where HDPE production kinetics are assumed to be first-order for ethylene concentration in a liquid and catalyst flow rate, wherein kinetic rate is determined by:

$$P_o = kc_o C_E \tau_s.$$

26. (New) The process of Claim 23, where catalyst activity is determined by:

$$p = \frac{P_o}{c_o}; \text{ and}$$

$$k = \frac{P}{\tau_s C_E} = \frac{1624.9 \text{ lb/lb}}{(45.9 \text{ min})(5.0537 \text{ wt}\%)} = 7.00 \text{ lb/lb/min/wt}\%;$$

where catalyst feed factor is a function of other measured reactor variables, making it independent of catalyst type or catalyst activity, expressed by:

$$f_c = kc_i, \text{ then}$$

using mass balance of a catalyst around the reactor and a rearranged kinetic rate equation to determine catalyst feed factor, by:

$$f_c = kc_i = kc_o = \frac{P_o}{\tau_s C_E} = \frac{58034 \text{ lb/h}}{(45.9 \text{ min})(5.0537 \text{ wt}\%)} = 250 \text{ lb/h/min/wt}\%,$$

where a catalyst activity factor quantifies reactivity of a specific catalyst with respect to its size, expressed as:

$$k_c = \frac{k}{d_c^3} = \frac{7.00 \text{ lb/lb/min/wt}\%}{(100\mu)^3} \cdot \frac{1e06 \text{ lb}}{1 \text{ MMlb}} = 7.00 \text{ lb/MMlb/min/wt}\%/\mu^3.$$